[振動分配関数]

$$q_{\mathrm{vib}}^{(1)} = \left[1 - \exp\left(-\frac{h\nu}{k_{\mathrm{B}}T}\right)\right]^{-1} \qquad \text{1 振動子} \quad (7.4)$$

$$q_{\mathrm{vib\text{-}cl}}^{(1)} = \frac{k_{\mathrm{B}}T}{h\nu} \qquad \text{古典極限 1 振動子} \quad (7.4\text{-cl})$$

$$q_{\mathrm{vib}} = \prod_{i=1}^{n_{\mathrm{v}}}\left[1 - \exp\left(-\frac{h\nu_i}{k_{\mathrm{B}}T}\right)\right]^{-1} \qquad n_{\mathrm{v}} \text{ 振動子} \quad (7.5)$$

[回転分配関数]

$$q_{\mathrm{rot}}^{2\mathrm{D}} = \int_0^{\infty} \rho_{\mathrm{rot}}^{2\mathrm{D}} \exp\left(-\frac{\varepsilon_J}{k_{\mathrm{B}}T}\right) \mathrm{d}\varepsilon_J = \frac{k_{\mathrm{B}}T}{\sigma B} \qquad \text{2 次元回転子} \quad (7.6)$$

σ: 回転対称数
= 2 (H_2, N_2, CO_2)
= 1 (HCl, N_2O)

$$q_{\mathrm{rot}}^{3\mathrm{D}} = \frac{n_{\mathrm{isom}}\pi^{1/2}}{\sigma}\left(\frac{k_{\mathrm{B}}T}{A}\frac{k_{\mathrm{B}}T}{B}\frac{k_{\mathrm{B}}T}{C}\right)^{1/2} \qquad \text{3 次元回転子} \quad (7.7)$$

σ: 回転対称数
= 2 (H_2O, SO_2)
= 3 (NH_3)
:

n_{isom} : (光学)異性体の数

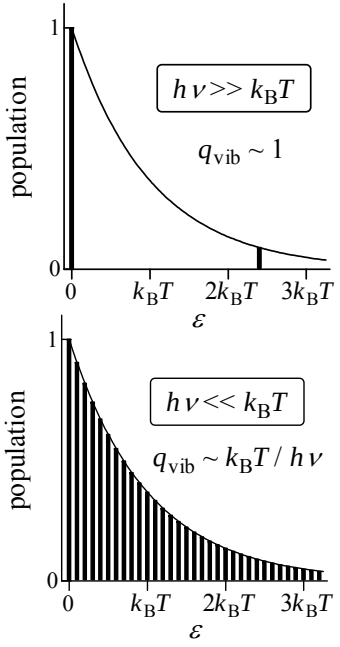
[並進分配関数]

$$q_{\mathrm{trans}}^{1\mathrm{D}} = \left(\frac{2\pi m k_{\mathrm{B}}T}{h^2}\right)^{1/2} l \qquad \text{1 次元並進} \quad (7.8)$$

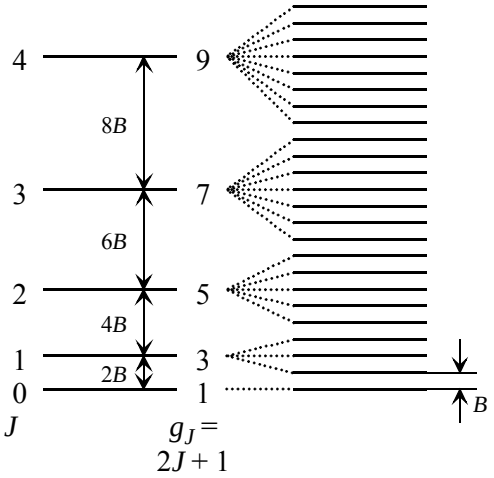
$$q_{\mathrm{trans}}^{3\mathrm{D}} = \left(\frac{2\pi m k_{\mathrm{B}}T}{h^2}\right)^{3/2} l_x l_y l_z \qquad \text{3 次元並進} \quad (7.9)$$

$$q_{\mathrm{trans}}^{\circ} = \left(\frac{2\pi m k_{\mathrm{B}}T}{h^2}\right)^{3/2} \qquad \text{3 次元並進/単位体積あたり} \quad (7.10)$$

$$q_{\mathrm{trans}}^{\circ} = \left(\frac{2\pi \mu k_{\mathrm{B}}T}{h^2}\right)^{3/2} \qquad \text{3 次元相対並進/単位体積あたり} \quad (7.11)$$

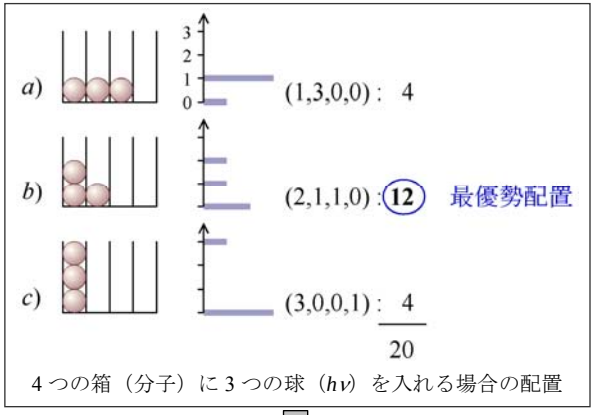


10.1 振動分配関数

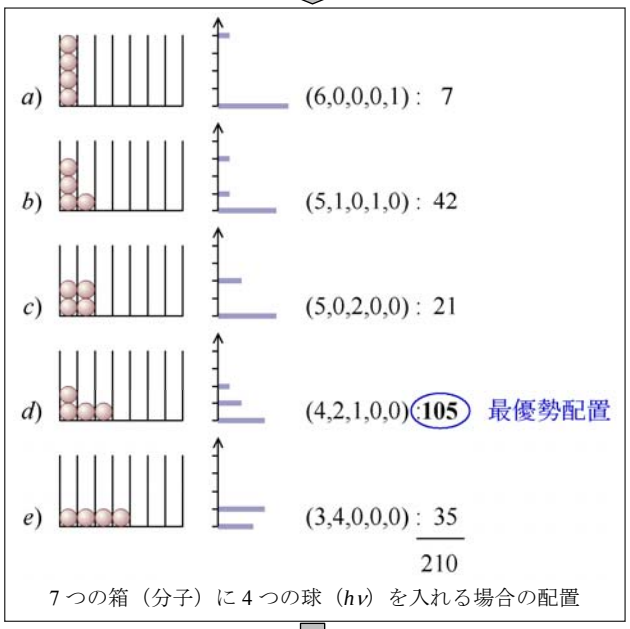


10.2 二次元回転の状態密度 $\sim 1 / B$

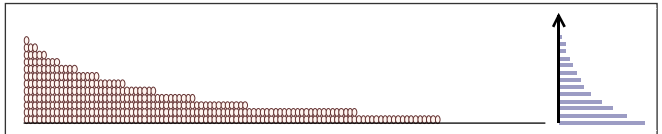
10.3 ボルツマン分布 – 統計力学的裏付



4 つの箱（分子）に 3 つの球（$h\nu$）を入れる場合の配置



7 つの箱（分子）に 4 つの球（$h\nu$）を入れる場合の配置



n 個の箱（分子）に m 個の球（$h\nu$）を入れる場合の最優勢配置